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The Structure of Amorphous Materials

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Massachusetts Institute of Technology  
Cambridge, Massachusetts 02139

Principal Investigator: B. L. Averbach  
(617) 864-6900 Ext. 3320

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## The Structure of Amorphous Materials

B. L. Averbach  
Professor of Metallurgy  
Massachusetts Institute of Technology

We are investigating the atomic arrangement in amorphous materials which are used as semiconductor switches.

Amorphous  $As_2Se_3$  has been selected as a typical threshold switch and amorphous  $Te_{85}Ge_{15}$  as a typical memory switch. Small amounts of Te and Sb are usually added to  $As_2Se_3$  to adjust the conductivity. In a similar way small amounts of As and Sb are usually added to  $Te_{85}Ge_{15}$  to improve the switching lifetime. We plan to investigate the structures with and without the alloy additions, but we anticipate that there will be little change in the atomic arrangement in the doped material.

It appears that there is considerable short range structure in these materials, and we hope to correlate this structure with the switching characteristics.

### Review of Progress

The atomic arrangement is being determined by means of an X-ray diffraction technique which has been developed in this laboratory. X-ray scattering curves are being obtained using  $RhK\alpha$  and  $CoK\alpha$  radiations. After corrections for Compton scattering and multiple scattering, the data are treated by

means of a computer method which provides corrections for systematic errors and termination effects. This method has been described in our paper on the structure of amorphous selenium.<sup>1</sup> The result of this procedure is a radial distribution curve which is free of false detail.

During the initial stages of our work, we have obtained the data for bulk amorphous  $As_2Se_3$ . A number of separate runs were required with each radiation and counting times were chosen so that the intensity was statistically significant to one percent at every point. This required prolonged counting at high scattering angles.

The data were obtained on a horizontal spectrometer with a LiF monochromator in the diffracted beam. An automatic step-counter was used and the data were recorded on paper tape. The paper tape was then used to generate the resultant scattering curve.

Our first corrections involved the evaluation of the Compton scattering and the normalization of the scattering. These procedures have been performed successfully, and we are now eliminating the termination errors. The resultant curve will be a corrected radial distribution function.

We will investigate the structure of the amorphous material by comparing with powder pattern data from crystalline

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<sup>1</sup> R. Kaplow, T. A. Rowe, and B. L. Averbach, "Atomic Arrangement in Vitreous Selenium", Phys. Rev., Vol. 168, No. 3, 1068-1079, 15 April 1968.

$\text{As}_2\text{Se}_3$ . We expect to introduce a Monte Carlo method to study the deviations from the crystalline structure. Alternatively we expect to start with a random collection of atoms and to use the Monte Carlo procedure to arrive at the final structure. We expect our final structure to be an atomic arrangement which is consistent with the measured radial distribution function.

Our work on the memory switch is just underway. We have prepared the composition  $\text{Te}_{85}\text{Ge}_{15}$  in bulk form. The material is crystalline and we expect to heat treat the compound in order to produce an amorphous structure. We intend to proceed in a similar fashion with the structure of the amorphous compound.

#### Plans for the Next Stage

We expect to continue with the X-ray diffraction work. The results for amorphous  $\text{As}_2\text{Se}_3$  should be in an advanced stage by the end of the first year. The work on  $\text{Te}_{85}\text{Ge}_{15}$  will not be as far along and we anticipate that these data will be in a reportable form in the early portion of the second year. We will then proceed with alloy additions which will bring these materials closer to the compositions used for practical switches.

During the second part of the first year, we intend to initiate our work on electron scattering through thin films of these materials. Our electron microscope is fitted with an energy selection system and we will use this to obtain

diffraction data from thin films. We will be able to compare the electron scattering with the X-ray data from the bulk materials, and we hope to characterize the defects present in the thin films.

We are in close contact with the program which is being carried out in Professor Adler's laboratory. The latter group is measuring the switching properties of these materials and we expect to make use of their data in interpreting our results.